

Information-theoretic vs. thermodynamic entropy production in autonomous sensory networks

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For sensory networks, we determine the rate with which they acquire information about the changing external conditions. Comparing this rate with the thermodynamic entropy production that quantifies the cost of maintaining the network, we find that there is no universal bound restricting the rate of obtaining information to be less than this thermodynamic cost. These results obtained within a general bipartite model consisting of a stochastically changing environment that affects the instantaneous transition rates within the system are illustrated with a simple four-states model motivated by cellular sensing. On the technical level, we obtain an upper bound on the rate of mutual information analytically and calculate this rate with a numerical method that estimates the entropy of a time-series generated with a simulation.

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Acquiring and processing information about the instantaneous state of the environment is a prerequisite for survival for any living system. Sensory and signal transducing networks have evolved to achieve this task under a variety of external conditions as, e.g., the work on bacteria like *Escherichia coli* has demonstrated so beautifully [1, 2]. Maintaining any biochemical network, however, has a metabolic cost associated with its inherent non-equilibrium nature. This fact prompts the question whether there is a relation between the performance of the network and its free energy consumption. For sensory adaptation in *E. coli*, such a trade-off between adaptation speed and accuracy, and the energy dissipation rate has recently been found in a theoretical model and confirmed with experimental data [3].

From a more information-theoretic perspective, the question alluded to above can be formulated more generally as to whether there is any quantitative relation between the rate with which such a network acquires information about the ever changing environmental conditions and the rate of entropy production associated with the functioning of the network. The universal concept for quantifying one side of this balance is mutual information, or, more precisely, the rate of mutual information. In the context of sensing, this rate has been introduced in [4], where it was explored for the special case of Gaussian input and output signals and various network motifs. Importantly, as pointed out in [4], because it takes temporal correlations into account the rate of mutual information is different from the static mutual information, which has been the subject of several recent investigations in genetic regulatory networks [5]. On the other hand, calculating the rate of mutual information without the assumption of Gaussian statistics represents a main challenge.

In this paper, we obtain an upper bound on the rate of mutual information for a general bipartite model consisting of an environment that switches stochastically between an arbitrary number of states and a network for

which the internal transition rates depend on the instantaneous state of the environment. This set-up has the advantage that the total system is in a non-equilibrium steady state generated by a Markovian dynamics which facilitates the analysis. Still, since the internal process is non-Markovian, deriving the expression for this bound as done below becomes non-trivial. Moreover, in order to calculate the precise value of the rate of mutual information we apply a numerical method that estimates the entropy rate of a single time-series produced from a numerical simulation [6–8]. For evaluating the second side of the balance introduced above, we need the rate of (thermodynamic) entropy production, as it has been derived for any network with given transition rates some time ago [9] and revitalized in the context of stochastic thermodynamics as reviewed in [10].

Significant progress in relating information-theoretic concepts to thermodynamic ones has recently been achieved in the context of feedback-driven systems [11–16]. For these systems, the amount of mutual information between system and controller enters the corresponding thermodynamic expressions on the level of generalized fluctuation theorems and second-law like inequalities. In particular, the net-power output of such systems can not exceed the rate of mutual information acquired. The single cell, however, is an autonomous system for which a separation into an act of measurement and subsequent feedback control does not come naturally. Whether despite this fundamental difference between a feedback-driven system and an autonomous one, an analogous constraint on a putative efficiency relating the rate of acquiring information with the thermodynamic cost of maintaining the sensory network exists will be explored here.

In order to introduce this rate of mutual information between external and internal processes and compare it to the entropy production, we first consider the minimalistic model shown in Fig. 1. The environment is sup-

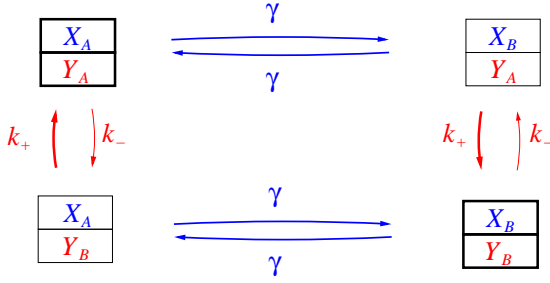


FIG. 1: Network and transition rates of a simple model of an internal process Y coupled to an external one X .

posed to switch stochastically with rate γ between two possible states X_A and X_B . Within the system, there is an internal degree of freedom, which exists also in two different states that are correlated with the environment state. Specifically, if the external state is X_A (X_B) and the internal state is in the “false” state Y_B (Y_A), the internal state changes to Y_A (Y_B) with a rate k_+ . We also allow for a (small) rate k_- inducing “false” transitions. Later we will consider a more realistic model for bacterial chemotaxis, where the external states correspond to the state of a receptor sitting on the membrane, while the internal states correspond to some internal protein that can be transformed to an active form with transition rates that depend on the state of the receptor.

As we will show below in equation (13) using a general framework, the rate \mathcal{I} at which the internal system acquires information about the time-dependent state of the environment is bounded from above by

$$\mathcal{I}^{(u)} = f(k_+, k_-) + f(k_-, k_+), \quad (1)$$

where $f(x, y) \equiv \frac{x(y+\gamma)}{2\gamma+x+y} \ln \frac{x(x+y+2\gamma)}{2xy+(x+y)\gamma}$. For $k_- = 0$ and in the limit $k_+ \gg \gamma$, the rate of mutual information can be understood as follows. The uncertainty about the external time-series $X(t)$ still left after recording the internal time-series $Y(t)$ is basically the specific time lapse between a change in the external conditions and the change of the internal state, since for $k_- = 0$ an internal jump takes place only after an external jump. Thus the system can localize the change in the external conditions within a time window of width $1/k_+$. Encoding the length of intervals between switching events on a scale $1/k_+$ requires a number of order k_+/γ , which carries $\ln(k_+/\gamma)$ units of information (measured throughout this paper using natural logarithms). Since these switching events take place with a rate γ , the rate of mutual information, for $k_- = 0$ and $k_+ \gg \gamma$, is $\mathcal{I} \simeq \gamma \ln \frac{k_+}{\gamma}$. Therefore, in this limit, the upper bound (1) gives the correct value of the rate of mutual information.

The dissipation rate σ associated with this network follows from the standard expression for Markovian processes, recalled in equation (16) below, which gives

$$\sigma = g(k_+, k_-) + g(k_-, k_+), \quad (2)$$

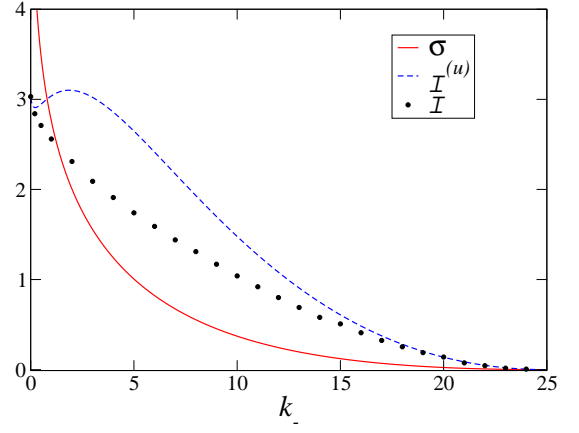


FIG. 2: The rate of mutual information \mathcal{I} , estimated with the numerical method explained in the text, the upper bound $\mathcal{I}^{(u)}$, and the thermodynamic entropy production σ as a function of k_- for $k_+ = 25$ and $\gamma = 1$. Here and in the following figures the common unit of time is arbitrary and the error in the numerics is less than the size of the symbols.

where $g(x, y) \equiv \frac{x(\gamma+y)}{2\gamma+x+y} \ln \frac{x}{y}$. The thermodynamic entropy production fulfills $\sigma \geq 0$ and is zero only if detailed balance is fulfilled ($k_- = k_+$).

Whereas the rate of mutual information is finite at $k_- = 0$, the entropy production diverges as $k_- \rightarrow 0$. Therefore, when the system is far from equilibrium ($k_- \ll k_+$) the dissipation rate is larger than the mutual information rate. On the other hand, at equilibrium ($k_- = k_+$) both quantities are zero: there is no dissipation and the internal and external processes are uncorrelated. Note that in this case also the internal process becomes Markovian. In Fig. 2 we compare the rate of mutual information obtained from numerical simulations, as explained below, with the thermodynamic entropy production. There is a value of k_- , which depends on k_+ and γ , beyond which the mutual information rate becomes larger than the thermodynamic entropy production. Thus, as our first main result, we have found that in the most simple conceivable model the rate of mutual information is not bounded by the dissipation rate.

We now address the problem of calculating the upper bound within a general bipartite model. It will be convenient to first treat time as discrete with a spacing τ . We denote the external states by α, β and their transition probabilities by $W^{\alpha\beta} \equiv w^{\alpha\beta}\tau$, where the transition is from α to β . The transition probability from the internal state i to the internal state j , given that the external state is α , is $W_{ij}^\alpha \equiv w_{ij}^\alpha\tau$. Hence, the transition probabilities of the internal transitions depend on the instantaneous external state. States of the total system are thus determined by the pair (α, i) , with the transition

probabilities of this full Markov process given by

$$W_{ij}^{\alpha\beta} \equiv \begin{cases} w^{\alpha\beta}\tau & \text{if } i = j \text{ and } \alpha \neq \beta \\ w_{ij}^{\alpha}\tau & \text{if } i \neq j \text{ and } \alpha = \beta \\ 0 & \text{if } i \neq j \text{ and } \alpha \neq \beta \end{cases}. \quad (3)$$

A stochastic trajectory with N jumps is denoted by $\{(X_t, Y_t)\}_{t=0}^{N\tau}$, where $\{X_t\}_{t=0}^{N\tau}$ ($\{Y_t\}_{t=0}^{N\tau}$) represents the external (internal) process. The information-theoretic entropy rate of the full process measures how much the entropy of the trajectory grows with N . In the limit $N \rightarrow \infty$, it is given by [17]

$$H_{X,Y} = -\frac{1}{\tau} \sum_{i,j,\alpha,\beta} P_i W_{ij}^{\alpha\beta} \ln W_{ij}^{\alpha\beta}, \quad (4)$$

where P_i^α denotes the stationary state probability distribution and, from equation (3), the diagonal terms take the form $W_{ii}^{\alpha\alpha} = 1 - \sum_{\beta \neq \alpha} w^{\alpha\beta}\tau - \sum_{j \neq i} w_{ij}^{\alpha}\tau$. Moreover, since the external transitions are independent of the internal degrees of freedom, the external process $\{X_t\}_{t=0}^{N\tau}$ is also Markovian, which implies for its entropy rate

$$H_X = -\frac{1}{\tau} \sum_{\alpha\beta} P^\alpha W^{\alpha\beta} \ln W^{\alpha\beta}, \quad (5)$$

where $P^\alpha = \sum_i P_i^\alpha$ and $W^{\alpha\alpha} = 1 - \sum_{\beta \neq \alpha} w^{\alpha\beta}\tau$. Here, we are interested in calculating the rate of mutual information defined as [17]

$$I_{X,Y} = H_X + H_Y - H_{X,Y}. \quad (6)$$

The still missing piece for evaluating this expression is the entropy rate of the internal process H_Y , which is not known because Y_t is in general non-Markovian. However, this quantity is bounded from above and from below by the relation [17]

$$H(Y_{n+1}|Y_n, \dots, Y_1, X_1) \leq H_Y \leq H(Y_{n+1}|Y_n, \dots, Y_1), \quad (7)$$

which involves conditional entropies. Here, we are considering a finite sequence of n jumps of the internal process starting with the stationary state probability distribution. These bounds become better as n increases and for $n \rightarrow \infty$ both converge to the same value which is the entropy rate H_Y [17]. The first upper bound is given by

$$H(Y_2|Y_1) = -\frac{1}{\tau} \sum_{Y_1} P(Y_1) \sum_{Y_2} P(Y_2|Y_1) \ln P(Y_2|Y_1). \quad (8)$$

Using the transition rates (3) we have

$$P(Y_2|Y_1) = \frac{\sum_{X_1} P(Y_2, Y_1, X_1)}{P(Y_1)} = \frac{\sum_{\alpha} P_i^\alpha w_{ij}^{\alpha}\tau}{P_i}, \quad (9)$$

where we substituted $X_1 \rightarrow \alpha$, $Y_1 \rightarrow i$, and $Y_2 \rightarrow j$. With this relation it is easy to obtain

$$H(Y_2|Y_1) = -\sum_{i,\alpha} P_i^\alpha \sum_{j \neq i} \left(w_{ij}^{\alpha} \ln \frac{\sum_{\beta} P_i^\beta w_{ij}^{\beta}\tau}{P_i} - w_{ij}^{\alpha} \right) + O(\tau) \quad (10)$$

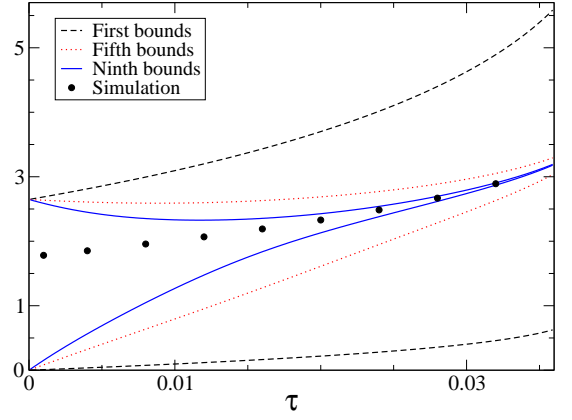


FIG. 3: The lower and upper bounds on the mutual information rate and the numerical simulation result as a function of τ for $k_- = 5$, $k_+ = 25$, and $\gamma = 1$. The simulations were done for a time series with $N = 10^{10}$.

Moreover, from (4) and (5), we get

$$H_X - H_{X,Y} = \sum_{i,\alpha} P_i^\alpha \sum_{j \neq i} (w_{ij}^{\alpha} \ln w_{ij}^{\alpha}\tau - w_{ij}^{\alpha}) + O(\tau). \quad (11)$$

Therefore, the first upper bound for the rate of mutual information, as obtained from (6), (10), and (11), reads

$$I_{X,Y}^{(u,1)} = \sum_{i,\alpha} P_i^\alpha \sum_{j \neq i} w_{ij}^{\alpha} \ln \frac{w_{ij}^{\alpha}}{\bar{w}_{ij}} + O(\tau), \quad (12)$$

where $\bar{w}_{ij} \equiv \sum_{\beta} P(\beta|i) w_{ij}^{\beta}$ is the mean internal transition rate and $P(\beta|i) = P_i^\beta / P_i$ is the probability of being in the external state β given that the internal state is i . More generally, we find that up to $O(\tau \ln \tau)$ all upper bounds with finite n are given by this expression, meaning that $I_{X,Y}^{(u,n)} = \sum_{i,\alpha} P_i^\alpha \sum_{j \neq i} w_{ij}^{\alpha} \ln \frac{w_{ij}^{\alpha}}{\bar{w}_{ij}} + O(\tau \ln \tau)$. As for the lower bounds, we find that $I_{X,Y}^{(l,n)} = O(\tau \ln \tau)$ for all n . Therefore, we conclude that the rate of mutual information in the continuous time limit is bounded from above by

$$\mathcal{I}^{(u)} = \sum_{i,\alpha} P_i^\alpha \sum_{j \neq i} w_{ij}^{\alpha} \ln \frac{w_{ij}^{\alpha}}{\bar{w}_{ij}}. \quad (13)$$

We note that all the bare entropy rates diverge as $\ln \tau$ for $\tau \rightarrow 0$ and, therefore, cannot be defined in this limit [18, 19]. However, the rate of mutual information is a well behaved quantity in this limit with no logarithmic divergences.

Let us now explain the numerical method we use to estimate the entropy rate H_Y of the non-Markovian time series $\{Y_t\}_{t=0}^{N\tau}$. The random matrix $\mathcal{T}(Y_t, Y_{t-1})$, is defined as $\mathcal{T}(Y_t, Y_{t-1})_{X_t, X_{t-1}} = P[Y_t, X_t | Y_{t-1}, X_{t-1}]$, where $P[Y_t, X_t | Y_{t-1}, X_{t-1}]$ is a conditional probability. If the external states take the values $X_t = 1, \dots, \Omega$, then \mathcal{T}

is a $\Omega \times \Omega$ matrix, where the internal variables (Y_t, Y_{t-1}) make the matrix random. It is simple to show that [6, 7]

$$P[\{Y_t\}_{t=0}^{N\tau}] = \mathcal{V} \mathcal{T}(Y_N, Y_{N-1}) \dots \mathcal{T}(Y_1, Y_0) \mathcal{P}_0 \quad (14)$$

where $P[\{Y_t\}_{t=0}^{N\tau}]$ is the probability of the time series, \mathcal{V} is a vector with all components equal to one and \mathcal{P}_0 is a vector with components $P(Y_0, X_0)$, for $X_0 = 1, \dots, \Omega$. From this relation, it is then possible to show that given a typical long time series $\{y_t\}_{t=0}^{N\tau}$, one can estimate the entropy rate H_Y by the formula [6–8]

$$H_Y \approx \frac{1}{N\tau} \ln \left\| \prod_{t=1}^N \mathcal{T}(y_t, y_{t-1}) \right\|, \quad (15)$$

where $\|\cdot\|$ is any matrix norm. Therefore, following Ref. [8], we can calculate H_Y numerically by generating an internal time-series with a simulation and calculating the above product by normalizing it after a certain number of steps (keeping track of the normalization factors), as explained in [20]. In Fig. 3, we plot upper and lower bounds on the mutual information rate, obtained from (7), and the numerical simulation result. For small τ , the numerically obtained rate of mutual information shows linear behavior, which we extrapolate to $\tau \rightarrow 0$ to estimate the rate of mutual information in the continuous time limit.

The other central physical observable we consider here is the thermodynamic entropy production [9, 10, 21], which for the present class of Markov processes reads

$$\sigma = \sum_{\alpha, \beta} P^\alpha w^{\alpha\beta} \ln \frac{w^{\alpha\beta}}{w^{\beta\alpha}} + \sum_{\alpha} \sum_{ij} P_i^\alpha w_{ij}^\alpha \ln \frac{w_{ij}^\alpha}{w_{ji}^\alpha}, \quad (16)$$

where the first term on the right hand side is due to the external transitions and the second is the contribution from internal transitions.

We finally use this framework to analyze a thermodynamically consistent minimal four-states model for bacterial chemotaxis in the spirit of the work of Berg and Purcell [2] (see also [22–25]). The external states are related to a receptor that can be either bound (on) by a ligand or empty (off). The transition from bound to empty happens at a rate k_{off} , whereas the binding rate k_{on} is proportional to the concentration of ligands in the external environment. The internal state is associated with a downstream protein that can be in an inactive (Y) or, due to phosphorylation, in an active state Y^* . For simplicity, we are assuming a two states internal system corresponding to one downstream protein. In reality, the number of downstream proteins is much larger than one [25], however, this simplification is not harmful for the qualitative comparison between the mutual information rate and thermodynamic entropy production.

The crucial coupling to the instantaneous state of the environment, here encoded by the state of the receptor, arises from the fact that the bound receptor speeds up

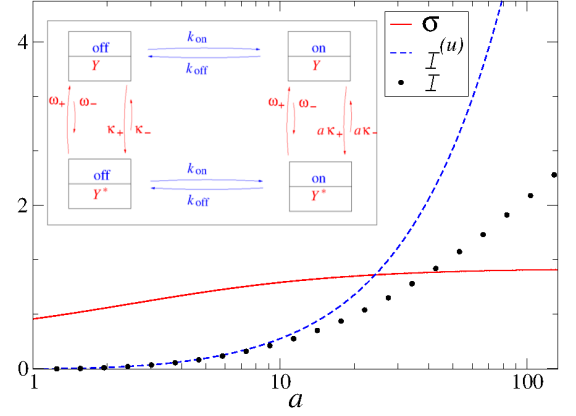
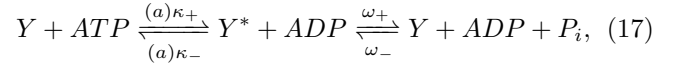


FIG. 4: The entropy production rate σ , the upper bound $\mathcal{I}^{(u)}$ and the numerically determined rate of mutual information \mathcal{I} as a function of a for the thermodynamically consistent model shown in the inset. The other parameters are set to $k_{\text{on}} = k_{\text{off}} = 1$, $\kappa_- = 1/10$, $\kappa_+ = 4/10$, $\omega_- = 1/10$, and $\omega_+ = 6/10$.

phosphorylation, which happens at a rate κ_+ , by a factor $a \geq 1$ compared to the action of an empty receptor. Dephosphorylation occurs at rate ω_+ , which leads to the following internal ATP consumption cycle



where the factor a arises only if the receptor is in the bound state. The full network of transitions is shown in Fig. 4. Thermodynamic consistency requires, first, that we also allow for the reverse transitions of phosphorylation and dephosphorylation with non-zero rates $(a)\kappa_-$ and ω_- , respectively. Second, it imposes a relation between the free energy associated with the ATP hydrolysis $\Delta\mu$ and the kinetic rates, which reads $\Delta\mu = k_B T \ln \frac{\kappa_+ \omega_+}{\kappa_- \omega_-}$, where k_B is Boltzmann's constant and T the temperature [9, 10].

In Fig. 4, we compare the rate of mutual information, obtained with the numerical simulation, with the rate of free energy consumption σ as a function of the enzymatic enhancement a . For $a = 1$, the internal state is decorrelated from the external one, leading to $\mathcal{I} = 0$. However, if $\Delta\mu \neq 0$, the internal network still consumes free energy. With increasing a the rate of mutual information increases, eventually becoming larger than the rate of free energy consumption. Thus, this thermodynamically fully consistent model confirms what we have found previously in the simple model: in such autonomous networks the rate of mutual information is not bounded by the free energy consumption required to maintain the network.

Why is the situation for an autonomous network apparently so different from what has been found for feedback-driven models? In the latter, information acquired through a measurement is used to extract net work from a thermal bath. The amount of net work

is limited by the information. Here, for the sensory network, we have investigated a complementary issue, namely whether the amount of information is limited by the chemical work, or free energy consumption, required to maintain the network. How this information is now used in a second step for an action that possibly performs work on some other element is an interesting but quite different question. As an important aside, we note that for an autonomous network the whole issue of writing the information into a memory whose erasure will require free energy [26, 27] is irrelevant as the erasure process is trivially included in the reaction scheme.

Clearly, these concluding remarks touch on deep issues concerning a future theory comparing comprehensively autonomous with feedback-driven systems which is a distinction that may become blurred in the micro world. On a more specific level, our study should now be refined by incorporating further elements of a more elaborate model of a sensory network, i.e., including several receptors, several proteins, allowing for adaptation and alike. The quantitative balance between information rate and entropy production will depend on such details, and thus, e.g., optimization of the “efficiency” will become an interesting issue. Searching for a hard universal thermodynamic bound for it, however, should be futile, as our simple model shows. Finally, an exact calculation of the rate of mutual information remains an open mathematical challenge.

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